Organic Geochemistry

The International Journal for the Rapid Publication of Current Research in Organic Geochemistry and Biogeochemistry

Editors-in-Chief
Earl W. Baker, *Florida*
A. G. Douglas, *Newcastle-upon-Tyne*

The Official Journal of the European Association of Organic Geochemists

List of Contents and Author Index

Volume 14 (1989)

PERGAMON PRESS
OXFORD • NEW YORK • BEIJING • FRANKFURT
SÃO PAULO • SYDNEY • TOKYO • TORONTO

European Association of Organic Geochemists

ORGANIC GEOCHEMISTRY

The Official Journal of the European Association of Organic Geochemists

Editors-in-Chief:

Dr Earl W. Baker, College of Science, Florida Atlantic University, Boca Raton, FL 33431, U.S.A.

Dr A. G. Douglas, Organic Geochemistry Unit, Drummond Building, University of Newcastle-upon-Tyne, Newcastle-upon-Tyne NE1 7RU, U.K.

Associate Editors

R. Alexander, Petroleum Geochemistry Group, School of Applied Chemistry, Curtin University of Technology, GPO Box U1987, Perth 6001, Western Australia, Australia
J. Connan, Elf-Aquitaine, CST Jean Feger, L2 109, Avenue Larribau, 64018 Pau Cedex, France
P. A. Cranwell, Freshwater Biological Association, The Ferry House, Ambleside, Cumbria LA22 0LP, U.K.
A. N. Fuex, Shell Development, P.O. Box 481, TX 77001, U.S.A.
A. Y. Huc, Institut Francais du Pétrole, BP 311 Rueil Malmaison 92506, France
K. Kvenvolden, U.S. Geological Survey, Menlo Park, CA 94025, U.S.A.
S. Larter, University of Oslo, Blindern, Oslo 3, Norway
G. W. M. Lijmbach, Shell Internationale Petroleum Maatschappi, E&P Division (EXP/34), P.O. Box 162, 2501 AN The Hague, The Netherlands
S. E. Palmer, AMOCO Production Company Research Center, 4502 East 41st Street, P.O. Box 3385, Tulsa, OK 74102, U.S.A.
M. Radke, KFA Jülich GmbH, P.O. Box 1913, D-5170 Jülich, F.R.G.
W. M. Sackett, University of South Florida, St Petersburg, FL 33701, U.S.A.
J. K. Whelan, Woods Hole Oceanographic Institution, Woods Hole, MA 02543, U.S.A.

Editorial Board

P. Albrecht, Université Louis Pasteur de Strasbourg, 67008 Strasbourg, France
M. Bjorøy, Geochemical Laboratories of Norway, P.O. Box 1581, 7001 Trondheim, Norway
G. E. Claypool, Mobil Research and Development Corp., 13777 Midway Road, Dallas, TX 75244, U.S.A.
J. M. Hayes, Biogeochemical Laboratories, Geology Building, Indiana University, IN 47405-5101, U.S.A.
J. M. Hunt, Woods Hole Oceanographic Institution, Woods Hole, MA 02543, U.S.A.
R. Ikan, Department of Organic Chemistry, Laboratory of Natural Products and Organic Geochemistry, The Hebrew University of Jerusalem, Jerusalem, Israel 91904
R. Ishiwatari, Tokyo Metropolitan University, Fukazawa 2-1-1, Setagaya-ku, Tokyo 158, Japan
Fu Jiamo, Institute of Geochemistry, Academia Sinica, Guiyang, Guizhou Province, People's Republic of China
D. Leythaeuser, KFA Jülich GmbH, P.O. Box 1913, D-5170 Jülich, F.R.G.
P. Meyers, Department of Geological Sciences, University of Michigan, 2024 C.C. Little Building, Ann Arbor, MI 48109, U.S.A.
A. A. Petrov, Institute of Geology and Exploitation of Combustible Minerals (IGiRGI), Oil Ministry, Academy of Sciences, 50 Fersman, Moscow 117312, U.S.S.R.
B. R. T. Simoneit, College of Oceanography, Oregon State University, Corvallis, OR 97331, U.S.A.
O. P. Strausz, Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada T6G 2G2
M. A. Wilson, CSIRO Division of Coal Technology, P.O. Box 136, North Ryde, NSW 2113, Australia

Members of the Board of EAOG

Professor P. A. Schenck—*Chairman*
Dr R. G. Schaefer—*Secretary* (KFA Jülich GmbH, Institute of Petroleum and Organic Geochemistry (ICH-5), P.O. Box 1913, D-5170 Jülich, F.R.G.)
Dr G. W. M. Lijmbach—*Treasurer*
Dr J. Connan Dr B. Durand Professor D. Leythaeuser Professor L. Mattavelli Dr K. Øygard

Publishing Office
Journals Production Unit, Pergamon Press plc, Hennock Road, Marsh Barton, Exeter, EX2 8NE, U.K. (*Tel.* Exeter (0392) 51558; *Telex* 42749)

Subscription and Advertising Offices
North America: Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523, U.S.A. *Rest of the World*: Pergamon Press plc, Headington Hill Hall, Oxford OX3 0BW, U.K. (*Tel.* Oxford (0865) 64881)

Subscription Rates
Annual institutional subscription rate (1990, Volumes 15 and 16) DM 1600.00; two-year institutional rate (1990/1991) DM 3040.00; personal subscription rate for those whose library subscribes at the regular rate DM 390.00. Prices are subject to amendment without notice.
Supplied to members of the European Association of Organic Geochemists as part of their membership dues. Members of the following societies can also purchase subscriptions at a concessional rate. Details of these rates are available on request.

Geochemical Society
International Association of Geochemistry and Cosmochemistry
Organic Geochemistry Division of the Geochemical Society
American Chemical Society
Meteoritical Society
American Association of Petroleum Geologists

Copyright © 1989 Pergamon Press plc. Published 6 issues/annum.

It is a condition of publication that manuscripts submitted to this journal have not been published and will not be simultaneously submitted or published elsewhere. By submitting a manuscript, the authors agree that the copyright for their article is transferred to the publisher, if and when the article is accepted for publication. However, assignment of copyright is not required from authors who work for organisations which do not permit such assignment. The copyright covers the exclusive rights to reproduce and distribute the article, including reprints, photographic reproductions, microfilm or any other reproductions of similar nature and translations. No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, electrostatic, magnetic tape, mechanical, photocopying, recording or otherwise, without permission in writing from the copyright holder.

Photocopying information for users in the U.S.A.
The Item-fee Code for this publication indicates that authorization to photocopy items for internal or personal use is granted by the copyright holder for libraries and other users registered with the Copyright Clearance Center (CCC) Transactional Reporting Service provided the stated fee for copying, beyond that permitted by Section 107 and 108 of the United States Copyright Law, is paid. The appropriate remittance of $3.00 per copy per article is paid directly to the Copyright Clearance Center Inc., 27 Congress Street, Salem, MA 01970 U.S.A. The Item-fee Code for this publication is 0146-6380/89 $3.00 + 0.00.

Permission for other use
The copyright owner's consent does not extend to copying for general distribution, for promotion, for creating new works, or for resale. Specific written permission must be obtained from the publisher for such copying.

Back issues
Back issues of all previously published volumes, in both hard copy and on microform are available direct from Pergamon Press offices.

♾™ The paper used in this publication meets the minimum requirements of American National Standard for Information Sciences—Permanence of Paper for Printed Library Materials, ANSI Z39.48-1984.

Number 1

Joseph A. Curiale and John R. Odermatt	1	Short-term biomarker variability in the Monterey Formation, Santa Maria Basin
H. Goossens, J. W. de Leeuw, W. Irene C. Rijpstra, G. J. Meyburg and P. A. Schenck	15	Lipids and their mode of occurrence in bacteria and sediments—I. A methodological study of the lipid composition of *Acinetobacter calcoaceticus* LMD 79–41
H. Goossens, R. R. Düren, J. W. de Leeuw and P. A. Schenck	27	Lipids and their mode of occurrence in bacteria and sediments—II. Lipids in the sediment of a stratified, freshwater lake
J. Martin E. Quirke, Lilia L. Cuesta, Richard A. Yost, Jodie Johnson and Edward D. Britton	43	Studies on high carbon number geoporphyrins by tandem mass spectrometry
Roger Sassen	51	Migration of crude oil from the Smackover source rock to Jurassic and Cretaceous reservoirs of the northern Gulf Rim
Mark A. McCaffrey, John W. Farrington and Daniel J. Repeta	61	Geochemical implications of the lipid composition of *Thioploca* spp. from the Peru upwelling region—15°S
Tanja Barth, Anne Eva Borgund and Anne Lise Hopland	69	Generation of organic compounds by hydrous pyrolysis of Kimmeridge oil shale—Bulk results and activation energy calculations
Alfred A. Christy, Anne Lise Hopland, Tanja Barth and Olav M. Kvalheim	77	Quantitative determination of thermal maturity in sedimentary organic matter by diffuse reflectance infrared spectroscopy of asphaltenes
Stuart G. Wakeham and Cindy Lee	83	Organic geochemistry of particulate matter in the ocean: The role of particles in oceanic sedimentary cycles
Richard A. Bourbonniere	97	Distribution patterns of dissolved organic matter fractions in natural waters from eastern Canada
Note		
F. Beach, T. M. Peakman, G. D. Abbott, R. Sleeman and J. R. Maxwell	109	Laboratory thermal alteration of triaromatic steroid hydrocarbons
Book Review		
Burtron H. Davis	113	"Catalysis in Coal Liquefaction: New Directions for Research" by Frank Derbyshire
Obituary	114	Peter H. Given 1918–1988
Reviewers for 1988	117	
Announcements	i	

Number 2

SELECTED PAPERS FROM THE SYMPOSIUM ON ORGANIC GEOCHEMISTRY: TECHNIQUES AND APPLICATIONS

194TH ACS NATIONAL MEETING

Editorial	V	
Guest Editorial	VI	
Gary J. Van Berkel, J. Martin E. Quirke and Royston H. Filby	119	The Henryville Bed of the New Albany shale—I. Preliminary characterization of the nickel and vanadyl porphyrins in the bitumen
Gary J. Van Berkel, J. Martin E. Quirke and Royston H. Filby	129	The Henryville Bed of the New Albany shale—II. Comparison of the nickel and vanadyl porphyrins in the bitumen with those generated from the kerogen during simulated catagenesis
Patrick G. Hatcher, Harry E. Lerch III, Anne L. Bates and T. Vincent Verheyen	145	Solid-state ^{13}C nuclear magnetic resonance studies of coalified gymnosperm xylem tissue from Australian brown coals
C. P. Antworth, R. R. Yates and W. T. Cooper	157	Applications of inverse chromatography in organic geochemistry—I. Characterization of polar solute–soil organic matter interactions by high performance liquid chromatography
H. Collazo-Lopez, R. R. Yates and W. T. Cooper	165	Applications of inverse chromatography in organic geochemistry—II. Measurement of solute activity coefficients in organic geopolymers by gas chromatography
Joseph E. Campana	171	Desorption ionization mass spectrometry and laser photodissociation of porphyrins and related compounds
R. P. Philp, C. A. Lewis, C. Campbell and E. Johnson	183	The ion trap detector as an aid to analytical chemists in the oil industry
Charles E. Bronnimann and Gary E. Maciel	189	^{1}H NMR spectra of coals of various rank, obtained by the CRAMPS technique
Aidalu Joubert Castro, Gary J. Van Berkel, Frank G. Doolittle and Royston H. Filby	193	Comparison of electron ionization and fast atom bombardment–mass spectrometry for the determination of nickel, vanadyl and free-base porphyrins
G. J. Van Berkel, G. L. Glish and S. A. McLuckey	203	Geoporphyrin structure determination using chemical ionization–mass spectrometry/mass spectrometry
Timothy D. Lash	213	Synthesis of the porphyrins from petroleum
Bob W. Wright and Richard D. Smith	227	Supercritical fluid chromatography–mass spectrometry: A potentially useful technique for porphyrin analysis
Announcements	i	

Number 3

A SELECTION OF PAPERS FROM THE 4TH ANNUAL MEETING OF THE SOCIETY FOR ORGANIC PETROLOGY

Editorial	V	
Introduction	VI	
M. H. Pytte	233	Comparison of Monterey Formation kerogens from the Salinas Basin and Santa Barbara area, California
Francis T. C. Ting and Jeffrey A. Sitler	247	Comparative studies of the reflectivity of vitrinite and sporinite
Y. Héroux, D. Michoux, M. Desjardins et D. Sangster	253	Pétrographie et géochimie des matières organiques des séquences plombo-zincifères d'âge Carbonifère, Bassin Salmon River, Nouvelle-Écosse, Canada
P. K. Mukhopadhyay	269	Characterization of amorphous and other organic matter types by microscopy and pyrolysis–gas chromatography
Scott A. Stout and William Spackman	285	Peatification and early coalification of wood as deduced by quantitative microscopic methods
James C. Hower	299	Petrology of liquefaction residues from the Breckinridge cannel, western Kentucky
Steven H. Poe, Darrell N. Taulbee and Robert A. Keogh	307	Density gradient centrifugation of −100 mesh coal: An alternative to using micronized samples for maceral separation
Sharon S. Crowley, Ronald W. Stanton and Thomas A. Ryer	315	The effects of volcanic ash on the maceral and chemical composition of the C coal bed, Emery Coal Field, Utah
Joan S. Esterle, John C. Ferm and Tie Yiu-Liong	333	A test for the analogy of tropical domed peat deposits to "dulling up" sequences in coal beds—Preliminary results
S. M. Rimmer, D. F. Bensley and J. C. Crelling	343	Fluorescence spectral analysis of sporinite in the Lower Kittanning coal bed
Note		
P. K. Mukhopadhyay, J. R. Gormly and J. E. Zumberge	351	Generation of hydrocarbons from the Tertiary coals of Texas—Coal as potential source rock for liquid hydrocarbons in a deltaic basin?
Addendum	353	
Announcements	i	

Number 4

R. M. Bustin, C. Link and F. Goodarzi — 355 — Optical properties and chemistry of graptolite periderm following laboratory simulated maturation

J. W. Smith, B. D. Batts and T. D. Gilbert — 365 — Hydrous pyrolysis of model compounds

Y. Lao, J. Korth, J. Ellis and P. T. Crisp — 375 — Heterogeneous reactions of 1-pristene catalysed by clays under simulated geological conditions

Roger Sassen, Chad McCabe, J. Richard Kyle and Elizabeth W. Chinn — 381 — Deposition of magnetic pyrrhotite during alteration of crude oil and reduction of sulfate

Caroline M. Preston, David E. Axelson, Marcel Lévesque, Sukhdev P. Mathur, Henri Dinel and Robert L. Dudley — 393 — Carbon-13 NMR and chemical characterization of particle-size separates of peats differing in degree of decomposition

Roderick J. Weston, R. Paul Philp, Carolyn M. Sheppard and Anthony D. Woolhouse — 405 — Sesquiterpanes, diterpanes and other higher terpanes in oils from the Taranaki Basin of New Zealand

Michael G. Strachan, Robert Alexander, Eddy A. Subroto and Robert I. Kagi — 423 — Constraints upon the use of 24-ethylcholestane diastereomer ratios as indicators of the maturity of petroleum

Fernando Alcazar, Mahlon C. Kennicutt II and James M. Brooks — 433 — Benthic tars in the Gulf of Mexico: Chemistry and sources

Jeffrey T. Gelwicks, J. Bruno Risatti and J. M. Hayes — 441 — Carbon isotope effects associated with autotrophic acetogenesis

R. P. Philp, Li Jinggui and C. A. Lewis — 447 — An organic geochemical investigation of crude oils from Shanganning, Jianghan, Chaidamu and Zhungeer Basins, People's Republic of China

J. D. Payzant, D. D. McIntyre, T. W. Mojelsky, M. Torres, D. S. Montgomery and O. P. Strausz — 461 — The identification of homologous series of thiolanes and thianes possessing a linear carbon framework from petroleums and their interconversion under simulated geological conditions

Note

Roger Sassen and Elizabeth W. Chinn — 475 — Effects of elemental sulfur during programmed pyrolysis of kerogen

Announcements — i

Number 5

Shuichi Yamamoto and Ryoshi Ishiwatari — 479 — A study of the formation mechanism of sedimentary humic substances—II. Protein-based melanoidin model

Shan-Tan Lu, Edward Ruth and Isaac R. Kaplan — 491 — Pyrolysis of kerogens in the absence and presence of montmorillonite—I. The generation, degradation and isomerization of steranes and triterpanes at 200 and 300°C

Shan-Tan Lu and Isaac R. Kaplan — 501 — Pyrolysis of kerogens in the absence and presence of montmorillonite—II. Aromatic hydrocarbons generated at 200 and 300°C

L. H. Lin, G. E. Michael, G. Kovachev, H. Zhu, R. P. Philp and C. A. Lewis — 511 — Biodegradation of tar-sand bitumens from the Ardmore and Anadarko Basins, Carter County, Oklahoma

N. A. Marley, P. Bennett, D. R. Janecky and J. S. Gaffney — 525 — Spectroscopic evidence for organic diacid complexation with dissolved silica in aqueous systems—I. Oxalic acid

M. R. Mello, E. A. M. Koutsoukos, M. B. Hart, S. C. Brassell and J. R. Maxwell — 529 — Late Cretaceous anoxic events in the Brazilian continental margin

C. Dubreuil, S. Derenne, C. Largeau, C. Berkaloff and B. Rousseau — 543 — Mechanism of formation and chemical structure of Coorongite—I. Role of the resistant biopolymer and of the hydrocarbons of *Botryococcus braunii*. Ultrastructure of Coorongite and its relationship with Torbanite

Jaap S. Sinninghe Damsté, Ernst R. van Koert, A. C. Kock-van Dalen, Jan W. de Leeuw and P. A. Schenck — 555 — Characterisation of highly branched isoprenoid thiophenes occurring in sediments and immature crude oils

Letter to the Editor
J. D. Saxby — 569 — Bolide impacts and their significance in fossil fuel geochemistry

Announcements — i

Number 6

X. Wang, I. Lerche and C. Walters — 571 — The effect of igneous intrusive bodies on sedimentary thermal maturity

G. M. Mason, L. G. Trudell and J. F. Branthaver — 585 — Review of the stratigraphic distribution and diagenetic history of abelsonite

Miryam Glikson, Kay Lindsay and John Saxby — 595 — *Botryococcus*—A planktonic green alga, the source of petroleum through the ages: Transmission electron microscopical studies of oil shales and petroleum source rocks

Anne L. Bates and Patrick G. Hatcher — 609 — Solid-state ^{13}C NMR studies of a large fossil gymnosperm from the Yallourn Open Cut, Latrobe Valley, Australia

G. E. Michael, L. H. Lin, R. P. Philp, C. A. Lewis and P. J. Jones — 619 — Biodegradation of tar-sand bitumens from the Ardmore/Anadarko Basins, Oklahoma—II. Correlation of oils, tar sands and source rocks

H. Rodger Harvey, Sean C. M. O'Hara, Geoffrey Eglinton and Eric D. S. Corner — 635 — The comparative fate of dinosterol and cholesterol in copepod feeding: Implications for a conservative molecular biomarker in the marine water column

G. Stojanova, M. D. Stefanova and M. Goranova — 643 — Fractional composition of neutral asphaltenes from disseminated organic matter in sedimentary rocks

Wilhelm Püttmann and Christian B. Eckardt — 651 — Influence of an intrusion on the extent of isomerism in acyclic isoprenoids in the Permian Kupferschiefer of the Lower Rhine Basin, N.W. Germany

C. B. Eckardt, M. Wolf and J. R. Maxwell — 659 — Iron porphyrins in the Permian Kupferschiefer of the Lower Rhine Basin, N.W. Germany

X. de las Heras, J. O. Grimalt, J. Albaigés, R. Julià and P. Anadon — 667 — Origin and diagenesis of the organic matter in Miocene freshwater lacustrine phosphates (Cerdanya Basin, Eastern Pyrenees)

Note

Jiasong Fang, Roger Sassen, Harry Roberts and Jeffrey Nunn — 679 — Organic geochemistry of sediments of the deep-water Gulf of Mexico Basin

Announcements — i